

n-Hexane
110-54-3 | DTXSID0021917

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.52×10^{-4} mol/L

Global applicability domain: Inside

Local applicability domain index: 8.33×10^{-1}

Confidence level: 8.73×10^{-1}

Nearest Neighbors from the Training Set

Image not found

n-Hexane

Measured: 1.10×10^{-4}

Predicted: 1.52×10^{-4}

Image not found

3-Methylpentane

Measured: 2.08×10^{-4}

Predicted: 2.39×10^{-4}

Image not found

2-Methylpentane

Measured: 1.72×10^{-4}

Predicted: 1.93×10^{-4}

Image not found

2,3-Dimethylbutane

Measured: 2.61×10^{-4}

Predicted: 2.72×10^{-4}

Image not found

2-Heptene

Measured: 1.53×10^{-4}

Predicted: 1.74×10^{-4}